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Silicon Based Heterojunction Devices For Microwave Amplification and Generation

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Abstract

Si-based heterojunction such as $Si/Si_{1-x}Ge_x$ offer a route to high speed devices on silicon substrates. F_{max}'s in excess of 150 GHz have been reported. [1] In this report we describe the first measurements of the effect of carbon the bandgap in defect-free $Si/Si_{1-x-y}Ge_xC_y$ films. The bandgap was measured by both transport and photoluminescence experiments. Adding carbon to compressively strained SiGeC films grown pseudormorphically on Si(100) was found to increase the bandgap by 21-26 meV/%C. This is far less than would occur by decreasing strain by just reducing the Ge content, and shows SiGeC can substantially expand the range of applications of Si-based heterostructures.

I. Introduction

The strain in pseudomorphic $Si_{1-x}Ge_x$ alloys on Si (100) substrates imposes a severe design constraint in heterojunction devices employing these layers. In concept, because C atoms are smaller than both Si and Ge atoms, C may be used to compensate the strain by adding it substitutionally to form $Si_{1-x-y}Ge_xC_y$ alloys. However, the solid solubility of C in Si is only about 1 ppm even at the melting point of Si; [2]. In spite of this, previous work has demonstrated that low-temperature, nonequilibrium epitaxy can produce $Si_{1-x-y}Ge_xC_y$ films with substitutional C concentrations greater than 2%. The bulk of this previous work has been of a structural nature, with reports of strain as a function of C concentration, for example [3]. To the best knowledge of the authors, however, prior to our work there was only one previous experimental report of a direct measurement of the bandgap of $Si_{1-x-y}Ge_xC_y$. Boucaud *et al.* reported 77 K photoluminescence (PL) spectra from $Si_{1-x-y}Ge_xC_y$ alloys with x=0.155 [4], but these spectra showed luminescence peaks assigned to dislocations, casting doubt on the strain condition of the films.

In this report, we describe photoluminescence spectra from pseudomorphic $Si_{1-x-y}Ge_xC_y$ alloys on Si (100) showing only band-edge, $Si_{1-x}Ge_x$-like PL with no dislocation lines or luminescent defects. The PL was measured between 2 and 77 K and showed band-edge $Si_{1-x}Ge_x$-like luminescence at all temperatures. We show that for a given bandgap, a larger critical thickness can be attained for films with C compared to those without C. Furthermore, from our experimental measurements of the bandgap of pseudomorphic $Si_{1-x-y}Ge_xC_y$ on Si (100), we calculated the bandgap of relaxed $Si_{1-x-y}Ge_xC_y$. It was found that the initial addition of C will tend to decrease the bandgap of unstrained $Si_{1-x-y}Ge_xC_y$ alloys. To confirm the luminescence is not just measuring a local minimum in bandgap, we also fabricated Si/SiGeC/Si npn HBT's, and used the HBT's to measure the effect of C on bandgap. This transport measurement measured the same bandgap as the PL measurements within experimental error.

The samples used in this work were grown by rapid thermal chemical vapor deposition (RTCVD) on Si (100) substrates at reduced pressure (6 Torr) [5]. All samples consisted of nominally undoped single, buried $Si_{1-x-y}Ge_xC_y$ layers. The $Si_{1-x-y}Ge_xC_y$ layers were deposited at 575°C from dichlorosilane, germane, and methylsilane in a hydrogen carrier, while the Si caps were deposited at 675°C from dichlorosilane. The samples received no thermal treatment after growth. There were two sets of samples: one with x=0.24, the other with x=0.38. SIMS confirmed layer thickness, flat C profiles, and that the Ge concentration was unchanged as methylsilane was added. For the rest of this report, quoted substitutional C concentrations were quantitatively determined from shifts in the (400) x-ray diffraction (XRD) peaks using a Ge:C strain compensation ratio of 8.3, [3] which corresponds to a strain reduction of - 0.0035/%C. The C concentrations measured by SIMS were consistently proportional to those measured by XRD but were significantly lower, opposite to what would be expected if some C was not substitutional. We associate the inconsistency between SIMS and XRD with poor SIMS calibration.

II. Bandgap Measurement of $Si_{1-x-y}Ge_xC_y$ by Photoluminescence

For the photoluminescence measurements, the excitation source was an argon laser with a pump power density of ~50 W/cm^2, and the detector was a liquid nitrogen-cooled Ge diode. Figure 1(a) shows PL spectra measured at 25 K from samples with x=0.38 and various C concentrations. These spectra are indeed $Si_{1-x}Ge_x$-like and exhibit no features other than the usual no-phonon (NP) and TO phonon replica peaks [6]. There was a clear blueshift in these band-edge PL features as the C content was increased, indicating that adding C tends to increase the bandgap of strained $Si_{1-x-y}Ge_xC_y$. As C was added the NP intensity increased relative to the TO intensity, suggesting enhanced alloy scattering due to the C atoms in the lattice. Also, note that the features in the 25 K spectra became narrower and weaker as C was added. This may have been due to reduced band filling [7] caused by a lower carrier lifetime in the samples with C. The spectra measured at 77 K were similar to those at 25 K, but were thermally broadened. Several samples were measured at 2 K as well, although the luminescence was weaker and the linewidth broader for unknown reasons [Fig. 1(b)].

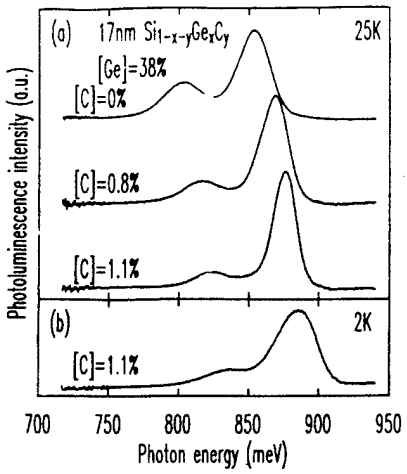

FIG. 1. Photoluminescence spectra for $Si_{1-x-y}Ge_xC_y$ samples with x=0.38 and various C levels. The pump power density was ~50 W/cm^2. The spectra were normalized and corrected to account for the spectral response of the experimental optical path.

To demonstrate the tradeoff between bandgap reduction and strain in $Si_{1-x}Ge_x$/Si heterojunction devices, we have plotted in Fig. 2 bandgap (as measured by PL) as a function of strain (as measured by XRD). The absolute bandgap of the control sample with x = 0.24 and y = 0 was determined from its 2 K PL spectrum. The bandgaps of the other samples were then determined by comparing the low-energy edge of the NP peak of their 77 K PL spectra to that of the control sample. We estimate error bars of $\pm$6 meV for the absolute bandgap measurements of $\pm$2 meV for the relative bandgaps.

The position of the $Si_{1-x-y}Ge_xC_y$ (4O) XRD peaks relative to the Si substrate peak were measured to give the vertical lattice constant of the epilayers. Assuming no relaxation (there was no evidence of significant dislocations in the PL spectra) and a Poisson ratio

of 0.28, the relaxed lattice constants and, therefore, the strain were computed. The relativity thin $Si_{1-x-y}Ge_xC_y$ layers (~30 nm) yielded broad XRD peaks, resulting in an estimated uncertainty in the strain of ± 0.0004.

Figure 2 shows bandgap versus biaxial compressive strain for both pseudomorphic $Si_{1-x}Ge_x$ on Si (100) (adapted from the work of Van de Walle and Martin [8]) and our experimental $Si_{1-x-y}Ge_xC_y$ data points. As C is added to $Si_{1-x}Ge_x$ and the Ge content is held fixed, the strain decreases and the bandgap increases, but the bandgap increase is much less than it would be if the strain was reduced simply by reducing the Ge concentration without adding C. That is, for a given bandgap, $Si_{1-x-y}Ge_xC_y$ has less strain (and presumably a greater critical thickness) than does $Si_{1-x}Ge_x$. The average slope of the $Si_{1-x-y}Ge_xC_y$ points, $\Delta E_G/\Delta\ \varepsilon$ = -6.1 eV/unit strain, corresponding to $\Delta E_G/\Delta y$ = +21 meV/%C. Furthermore, if one assumes a linear extrapolation of our $Si_{1-x-y}Ge_xC_y$ data to zero strain, one predicts a significant bandgap offset to Si for strain-free $Si_{1-x-y}Ge_xC_y$ films. For x = 0.38, the offset would be ~190 meV.

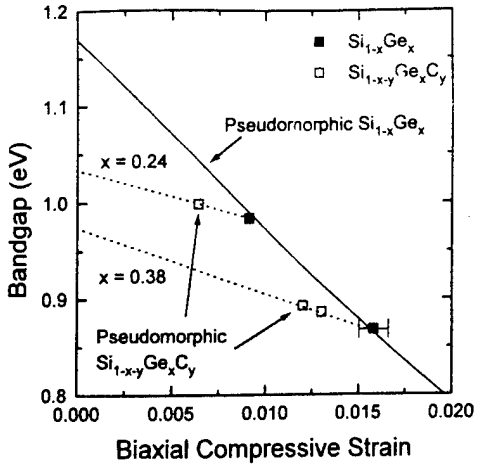

FIG. 2. Bandgap as a function of strain for pseudomorphic $Si_{1-x-y}Ge_xC_y$ on Si (100). The errors bar for relative bandgaps and strain are ± 2 meV and ± 0.0004, respectively. The $Si_{1-x}Ge_x$ line is from Ref. 10.

To demonstrate that adding C to $Si_{1-x}Ge_x$ can indeed increase its critical thickness, we prepared two samples under identical conditions (x = 0.38, thickness = 34 nm, and capped with 10 nm of Si), except that in one case we added C to the $Si_{1-x}Ge_x$ layer. The sample without C showed luminescence originating from dislocations [9] (Fig. 3), indicating that the sample was relaxed. The sample with C, however, showed only band-edge, $Si_{1-x}Ge_x$-like PL with no dislocation lines. By adding C to $Si_{1-x}Ge_x$, we achieve a strained film thicker than 30 nm with a band-offset to Si of almost 300 meV. In comparison, the Matthews-Blakeslee equilibrium critical thickness for a comparable $Si_{1-x}Ge_x$ film is ~7 nm [10].

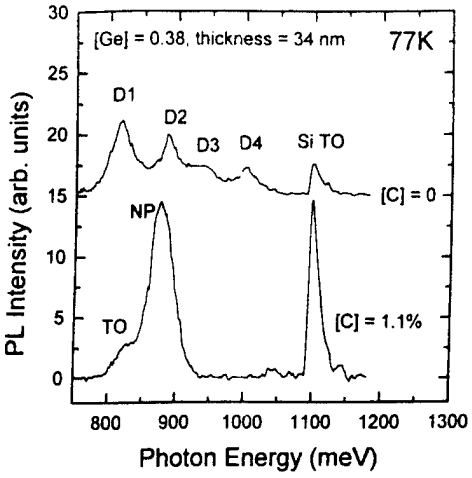

FIG. 3. Uncorrected photoluminescence spectra for two $Si_{1-x-y}Ge_xC_y$ samples with x = 0.38. For the top spectrum, y = 0; whereas for the bottom spectrum, y=0.011.

The substitutional incorporation of C into pseudomorphic $Si_{1-x}Ge_x$ should have two effects on the bandgap of the alloy. First, the smaller C atoms will reduce the strain in the film, thus increasing the bandgap. Additionally, the presence of C in the matrix should have a separate effect on the bandgap of the *relaxed* alloy. However, there are no published experimental results on the effect of small amounts of C on the bandgap of relaxed $Si_{1-y}C_y$ or $Si_{1-x-y}Ge_xC_y$, and theoretical predictions vary widely from +18 meV/%C [11] to ~ -100 meV/%C.[12] To subtract the expected effect of strain reduction from our experimentally measured bandgaps of strained layers, we assumed that the deformation potentials in our pseudomorphic $Si_{1-x-y}Ge_xC_y$ are similar to those in $Si_{1-x}Ge_x$ (ΔE_G = -11.7 eV/unit biaxial compressive strain) [8]. In Fig. 4 we have plotted the expected bandgap of relaxed $Si_{1-x-y}Ge_xC_y$ as a function of lattice constant. Note that the relaxed $Si_{1-x-y}Ge_xC_y$ points lie below the relaxed $Si_{1-x}Ge_x$ line [13] and, more importantly, that their slope is positive (~10 eV/nm). That is, as C is added and the lattice constant decreases, the relaxed bandgap does as well (-20 meV/%C). This is slightly surprising in light of the fact that SiC and diamond have bandgaps much larger than both Si and $Si_{1-x}Ge_x$. However, it is not unprecedented; similar "bowing" is observed or predicted in the bandgap versus lattice constant data of other alloy systems which have a large lattice mismatch (e.g. GaAs/GaSb and GaAs/GaN) [14].

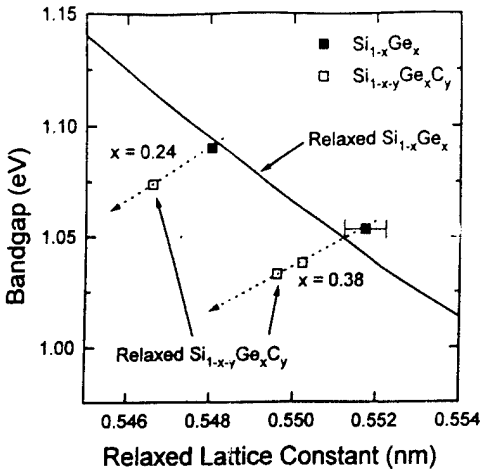

Fig. 4. Bandgap as a function of lattice constant for unstrained material. The $Si_{1-x-y}Ge_xC_y$ points are adapted from measuremnets on pseudomorphic films. The $Si_{1-x}Ge_x$ line is from Ref. 16.

Extrapolating our $Si_{1-x-y}Ge_xC_y$ data back to zero strain (Fig. 2) gives the bandgap of relaxed $Si_{1-x-y}Ge_xC_y$. This can then be compared to the known bandgap of the relaxed $Si_{1-x-y}Ge_xC_y$ alloy with the same Ge content to determine the effect of C on the bandgap of relaxed films. Doing so, we found that for *relaxed* $Si_{1-x-y}Ge_xC_y$, $\Delta E_G/\Delta y$ = -19 meV/%C. That this agrees with the above result (which assumed $Si_{1-x}Ge_x$ deformation potentials) confirms that the deformation potentials of $Si_{1-x-y}Ge_xC_y$ are indeed similar to those of $Si_{1-x}Ge_x$.

Note that our indirect fundamental bandgap results are consistent with those of ellipsometry and electroreflectance measurements of the direct optical transitions (3-5 eV) in pseudomorphically strained $Si_{1-y}C_y$ alloys [15,16]. Zollner *et al.* showed that the use of linearly interpolated transition energies and Si deformation potentials overestimated the E_0' transition energy as C was added, suggesting a downward trend in the bandgaps of relaxed $Si_{1-y}C_y$ and $Si_{1-x-y}Ge_xC_y$ alloys.

III. Bandgap Measurement of $Si_{1-x-y}Ge_xC_y$ by Heterojunction Bipolar Transistors

Fig. 5 shows a SIMS profile measured at Motorola of the following layer structure grown at Princeton. A 5 μm p^+ buffer layer was grown on p-type, 20 Ω cm, 100 mm wafers at 1000°C, followed by the 6000 Å, n^- collector doped with phosphorus between 10^{16} and 10^{17} cm^{-3}. The 460 Å, 7 x 10^{19} cm^{-3} doped $Si_{0.739}Ge_{0.25}C_{0.011}$ base was grown at 550°C with ~70 Å $Si_{0.739}Ge_{0.25}C_{0.011}$ undoped spacer layers on each side. The 600 Å, 8 x 10^{18} cm^{-3} doped emitter was then grown at 700°C followed by a 800 Å, 2 x 10^{19} emitter contact layer. XTEM performed at Motorola showed no defects, dislocations, or SiC precipitates in any of the 550°C layers. The 625°C structure was similar to the 550°C one, except that the base doping was an order of magnitude lower and the lightly doped collector was 2000 Å.

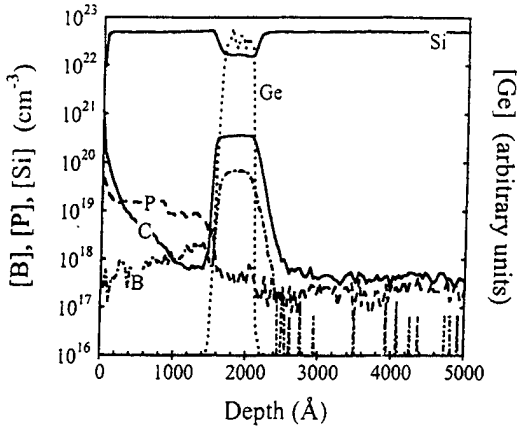

Fig 5. SIMS of a 1.1% carbon wafer showing B, P, Ge, Si, and C profiles. B and P are calibrated on a logarithmic scale. The C measurement is also plotted on a logarithmic scale with 7 orders of magnitude, but is not absolutely calibrated. Ge is plotted in arbitrary units on a linear scale.

Fig. 6 shows X-ray diffraction spectra from Princeton of the [004] reflections from the four wafers and bases grown at 550°C. Two peaks are present from each layer because the X-ray diffractometer did not filter out the $K_{\alpha 2}$ X-ray line. As carbon is added, note that the peaks of the strained $Si_{1-x-y}Ge_xC_y$ layers shift toward the Si substrate peak, indicating a reduction of strain. A shift in the X-ray peak ($\Delta 2\theta$) from the substrate of 1.4° was measured for the control sample, corresponding to x = 0.25. In the samples with carbon, it was assumed that the germanium levels did not change as C was added since the germane flow was held constant. This was confirmed by SIMS.

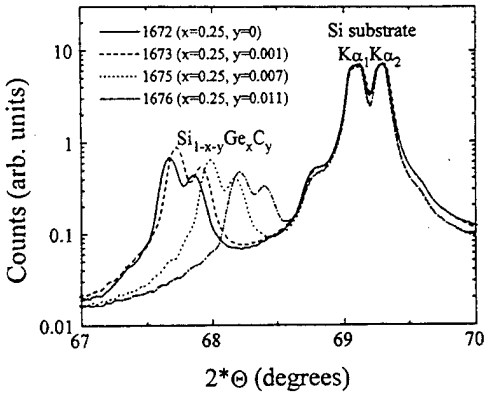

Fig. 6. X-ray diffraction spectra of the 550°C $Si_{0.75}Ge_{0.25}$ sample and the three 550°C $Si_{1-x-y}Ge_xC_y$ samples.

Carbon fractions of 0.1%, 0.7%, and 1.1% were extracted from the wafers with carbon, assuming that all carbon atoms were substitutional on lattice sites and that one substitutional carbon atom compensates 8.3 germanium atoms [17]. These carbon fractions correspond to strain compensation of 3%, 23%, and 37%, respectively. A Ge

fraction of 20% and carbon fractions of 0.45%, 0.55%, and 0.9% were extracted from the X-ray data for the wafers with bases grown at 625°C.

Large area devices were fabricated using a simple double mesa process. The base was revealed by a selective wet etch which defined the emitter-base junction area, while the collector-base junction was defined by dry etching a larger mesa around the emitter-base mesa. While this process leaves the emitter-base surfaces unpassivated, leading to large, non-ideal base currents, the process is adequate for measuring the ideal collector currents needed to measure changes in bandgap. Devices are easily and quickly fabricated by this process, and it has been used to demonstrate high frequency SiGe HBT's [18].

Fig. 7 shows the room-temperature common-emitter characteristics for both the 550°C and $Si_{0.75}Ge_{0.25}$ and the $Si_{0.743}Ge_{0.25}C_{0.007}$ devices with emitter areas of 900 μm^2. The control device shows a maximum h_{fe} of 40 while the 0.7% carbon device had a gain of 7.5. The collector-emitter breakdown voltage was ~15 V with $I_B = 0$ (and $I_C = 0$), but decreased to ~6 V with $I_C \sim 2$ mA, reflecting the fact that the gain was a function of bias. The large Early voltages (>300 V) indicate the absence of parasitic barriers which would be caused by base dopant outdiffusion [19,20]. From the curve-tracer figure, it is not possible to determine at fixed V_{BE} whether the decrease in gain between the control sample and the sample with carbon is due to a decrease in collector current or an increase in base current.

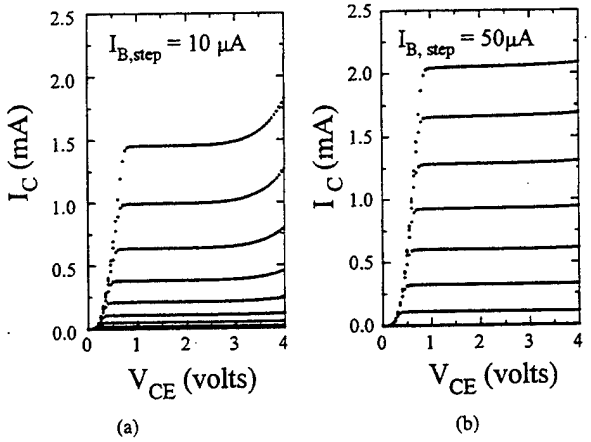

Fig. 7. Room-temperature common-emitter characteristics of the (a) 550°C $Si_{0.75}Ge_{0.25}$ and (b) $Si_{0.743}Ge_{0.25}C_{0.007}$ devices with emitter areas of 900 μm^2.

Fig. 8 shows room-temperature Gummel plots for the 625°C control device as well as for the 0.45%, 0.55% and 0.9% C devices for $V_{BC} = 0$. Note that the collector current has a slope of 60 meV/decade at room temperature, as expected for ideal collector currents in a bipolar transistor. The collector currents of devices with different perimeter to area ratios scale with emitter-base area. As the carbon level is increased, note the slight decrease in

I_C. Assuming no change in conduction and valence band density of states, base minority-carrier diffusion coefficient, and the base Gummel number, this shift indicates an increase in base bandgap as carbon is added. The base currents are nonideal, and measurements of $Si_{1-x}Ge_x$ devices with different perimeter to area ratios indicated that this base current scaled roughly with emitter-base perimeter. This should be expected due to the unpassivated transistor structure. In addition, above V_{BE} = 0.5 V, the devices show a clear increase in base current with increasing carbon fraction, leading to a decrease in transistor gain. The origin of this base current is under further study and may be related to decreasing minority carrier lifetime in the $Si_{1-x-y}Ge_xC_y$, possibly due to an impure methylsilane source. The Gummel plots for the 550°C base samples were similar, although I_B was somewhat higher at low current levels.

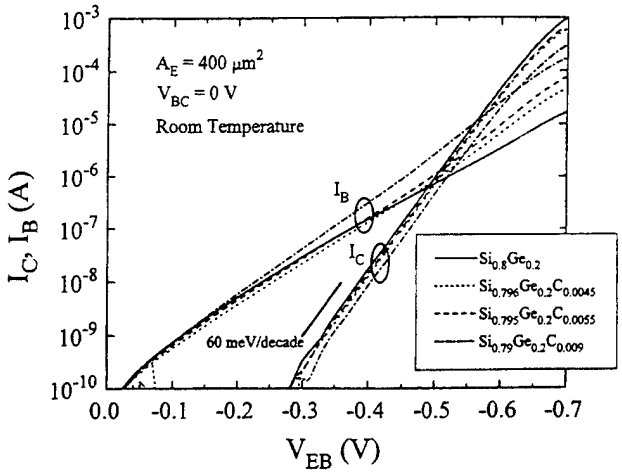

Fig. 8. Room-temperature Gummel plots of the 625°C control device and the 0.45%, 0.55%, and 0.9% carbon devicec.

It is well known that the difference in bandgap between the base regions of two HBT's may be extracted from the depends of their collector currents on temperature [21]. The ratio of collector currents in HBT's with different base compositions is

$$\frac{I_{C1}}{I_{C2}} = \frac{N_{G2}}{N_{G1}} \frac{(N_c N_v)_1}{(N_c N_v)_2} \frac{D_{n1}}{D_{n2}} e^{\Delta E_A / kT}$$

Where N_{Gi} is the base Gummel number, $(N_cN_v)_i$ is the product of the effective conduction and valence band densities of states, and D_{ni} is the electron diffusion coefficient. If there are no parasitic barriers in the conduction band, such as those resulting from conduction band offsets (ΔE_c) in abrupt junction devices without undoped spacer layers [22], or those resulting from base outdiffusion into the emitter and collector layers [23, 24], then the activation energy is the change in bandgap between the two materials, ΔE_g. This no-barrier assumption is justified in our case since $\Delta E_c \sim 0$ in the Si/strained $Si_{1-x}Ge_x$ system

[25] and because the undoped spaces in our devices would prevent any barrier formation from small amounts of boron diffusion or due to any small ΔE_c induced by carbon. The 550°C devices' high Early voltages (>300 V) and identical collector currents in forward and reverse made support this assumption.

Forward-active Gummel plots were measured from 180 to 350 K. Fig. 9 shows the ratio of I_{cSiGeC}/I_{cSiGe} at V_{BE} = 0.55 V as a function of inverse temperature for the 625°C transistors. Assuming a similar temperature dependence of electron diffusion coefficients and densities of states between the two samples, ΔE_g was then extracted from the slope of the lines. As seen from the graph, carbon incorporation clearly leads to an increased bandgap. Fig. 10 shows the change in bandgap versus carbon percentage for devices with both $x = 0.5$ and $x = 0.25$. The best fit is +26 meV/%C. This data is much more reliable than our preliminary results showing a near zero dependence on C [26]. In this work, a wider temperature measurement range was used, the temperature of the cold finger was measured more accurately, and higher quality expitaxial layers led to better collector current ideality factor (n ranged from 0.995 to 1.005 for all carbon fractions over the entire temperature range). Also note that there is no substantial difference in bandgap between 625°C and 550°C films.

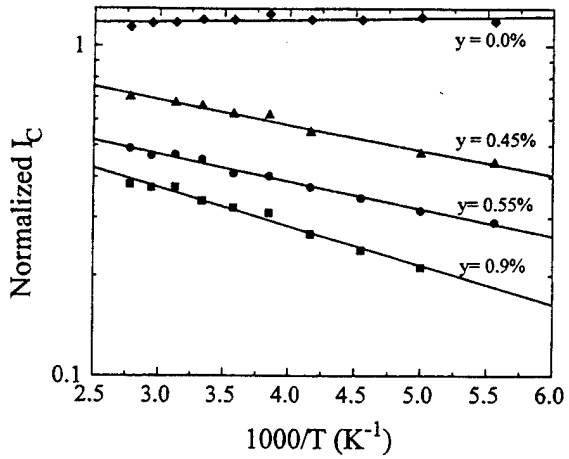

Fig. 9. Normalized collector current, ($I_{C,SiGeC}/I_{C,SiGe}$) versus inverse temperature for the 625°C devices with 0.0%, 0.45%, 0.55%, and 0.9% C

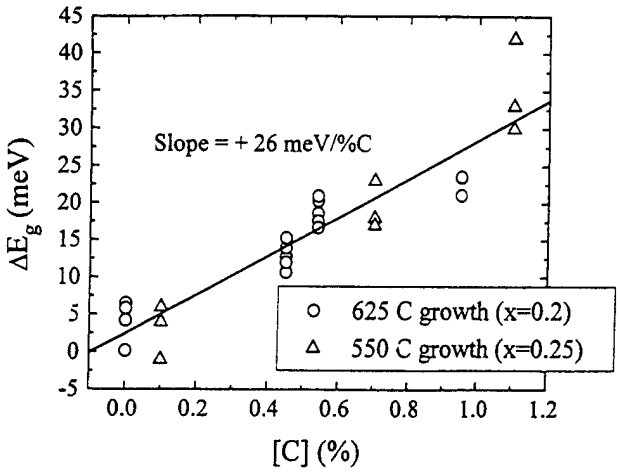

Fig. 10. ΔE_g as a function of carbon fraction for 625°C and 550° devices and the best linear fit to all devices measured.

IV. Summary

The effect of C on the bandgap of pseudomorphically strained $S_{1-x-y}Ge_xC_y$ alloys has been measured by photoluminescence (PL) in the range of x = 0.25-0.38 and y =0.0-0.0085 [27]. The measured changes in bandgap were 21-24 meV/%C. That our transport measurement yields a similar result, +26 meV/%C, is significant, since in SiGeC strong relaxation around C sites is known to occur [28]. This relaxation has been theoretically associated with a reduced bandgap [29]. If the bandgap was locally lower near C atoms, PL (which measures the recombination energy of an isolated exciton) might measure a lower bandgap than HBT transport measurements, where carriers much move through materials. That this did not occur suggest that the bandgap is spatially uniform.

Adding C (and keeping Ge fixed) to reduce the strain in pseudomorphic $Si_{1-x-y}Ge_xC_y$ alloys on Si, increases the bandgap by less than half the amount which would occur if the strained were reduced by lowering the Ge content alone. Therefore, to achieve a given bandgap less than that of Si, SiGeC alloys will have less strain than SiGe alloys and, furthermore, an increased thermal stability has been observed by structural photoluminescence measurements [30]. Therefore, SiGeC films should have technological uses since it overcomes the bandgap offset vs Si critical thickness trade-off which has limited the field for over 10 years. Finally, our work shows that fully compensated strain-free $Si_{1-x-y}Ge_xC_y$ layers on Si are expected to have a bandgap much lower than that of silicon.

V. References

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VI. Students Supported

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VII. Patents Filed

None

VIII. Publications Supported by this Grant

1. J.C. Sturm, A. St. Amour, Y. Lacroix, and M.L.W. Thewalt, "Deep photoluminescence in Si/$Si_{1-x}Ge_x$/Si quantum wells created by ion implantation and annealing," Appl. Phys. Lett. **64**, 2291-2293 (1994).

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IX. Conference Presentations Supported By This Grant

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